

1. Record Nr.	UNINA9911022160603321
Autore	Pal Sourav
Titolo	Theoretical Methods, Algorithms, and Applications of Quantum Systems in Chemistry, Physics, and Biology : Selected Proceedings of QSCP-XXVI Conference (Jaipur, India, October 2023) // edited by Sourav Pal, Vipin Srivastava, Vidya Avasare, Jean Maruani
Pubbl/distr/stampa	Cham : , : Springer Nature Switzerland : , : Imprint : Springer, , 2025
ISBN	3-031-85167-6
Edizione	[1st ed. 2025.]
Descrizione fisica	1 online resource (501 pages)
Collana	Progress in Theoretical Chemistry and Physics, , 2215-0129 ; ; 35
Altri autori (Persone)	SrivastavaVipin AvasareVidya MaruaniJean
Disciplina	530.12
Soggetti	Chemistry, Physical and theoretical Chemistry - Data processing Quantum chemistry Atoms Molecules Theoretical Chemistry Computational Chemistry Quantum Chemistry Atomic, Molecular and Chemical Physics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Part I. General Theory and Methodology -- Open Systems and the Laws of Thermodynamics -- Numerical Tensor Methods with Explicitly Correlated Wave Functions for Bound-State Stability of Coulomb Three-Body Systems -- P,T-Odd Sensitivity Parameters in Open-Shell Molecules from Relativistic Coupled-Cluster Theory -- Hypotheses on Many-Body Quantum Effects in Photosynthesis -- Revisiting Noble-Gas Adsorption on Graphene Using Continuum and Atomistic Descriptions -- From Quantum Connectivity to Biological Networks: A Portrait of Protein Structure seen through the Lens of Side Chain Network -- Part II. Computational Quantum Chemistry -- Insight into the Structural,

Electronic, and Magnetic Properties of Mn, Fe, and Co-doped bilayerborophene -- Deciphering the Mechanisms and Reactivity of Metalloenzymes and Biomimetic Models Using Computational Methods -- Dispersion effects on the computed geometries and properties of hydroxybenzenes dimmers -- Towards ML- and QML-Accelerated Discovery of Catalytic Materials and Mechanisms: A Progress Review -- Part III. Reaction Mechanisms -- Exploring the Competition between Energy Transfer and Reaction Rate in Post-TS Dynamics of Catechol's Ozonolysis -- Radical Pair Mechanism in Biological Systems -- Part IV. Biological Applications -- The Changing Face of Drug and Materials Discovery -- Understanding the Melanin Spectra and Photophysics -- Computational analysis of mutation effect on SARS-CoV-2 spike protein structures.

---

#### Sommario/riassunto

This volume contains peer-reviewed contributions based on talks presented at the 26th International Workshop on Quantum Systems in Chemistry, Physics, and Biology held in Jaipur, India, in October 2023. It provides an in-depth discussion of methodological approaches that are relevant across various length scales, elucidating their applications in diverse chemical and biological systems, such as catalysis and materials. Authored by experts in their respective fields, each chapter showcases recent developments and offers insights into the latest research trends. This book is aimed at advanced graduate students, academics, and researchers, both in university and corporation laboratories, interested in state-of-the-art and novel trends in quantum chemistry, physics, and biology, and their applications.

---